Linear Algebra

and its applications

FOURTH EDITION

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6.4 THE GRAM–SCHMIDT PROCESS

The Gram–Schmidt process is a simple algorithm for producing an orthogonal or orthonormal basis for any nonzero subspace of $\mathbb{R}^n$. The first two examples of the process are aimed at hand calculation.

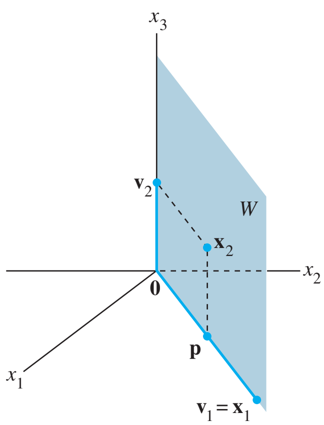


FIGURE 1
Construction of an orthogonal basis $\{\mathbf{v}_1, \mathbf{v}_2\}$.

EXAMPLE 1 Let $W = \text{Span}\,\{\mathbf{x}_1, \mathbf{x}_2\}$, where $\mathbf{x}_1 = \begin{bmatrix} 3 \\ 6 \\ 0 \end{bmatrix}$ and $\mathbf{x}_2 = \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix}$. Construct an orthogonal basis $\{\mathbf{v}_1, \mathbf{v}_2\}$ for W.

SOLUTION The subspace W is shown in Fig. 1, along with $\mathbf{x}_1$, $\mathbf{x}_2$, and the projection $\mathbf{p}$ of $\mathbf{x}_2$ onto $\mathbf{x}_1$. The component of $\mathbf{x}_2$ orthogonal to $\mathbf{x}_1$ is $\mathbf{x}_2 - \mathbf{p}$, which is in W because it is formed from $\mathbf{x}_2$ and a multiple of $\mathbf{x}_1$. Let $\mathbf{v}_1 = \mathbf{x}_1$ and

$$\mathbf{v}_2 = \mathbf{x}_2 - \mathbf{p} = \mathbf{x}_2 - \frac{\mathbf{x}_2 \cdot \mathbf{x}_1}{\mathbf{x}_1 \cdot \mathbf{x}_1}\mathbf{x}_1 = \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix} - \frac{15}{45}\begin{bmatrix} 3 \\ 6 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 2 \end{bmatrix}$$

Then $\{\mathbf{v}_1, \mathbf{v}_2\}$ is an orthogonal set of nonzero vectors in W. Since $\dim W = 2$, the set $\{\mathbf{v}_1, \mathbf{v}_2\}$ is a basis for W. ■

The next example fully illustrates the Gram–Schmidt process. Study it carefully.

EXAMPLE 2 Let $\mathbf{x}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$, $\mathbf{x}_2 = \begin{bmatrix} 0 \\ 1 \\ 1 \\ 1 \end{bmatrix}$, and $\mathbf{x}_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}$. Then $\{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3\}$ is clearly linearly independent and thus is a basis for a subspace W of $\mathbb{R}^4$. Construct an orthogonal basis for W.

SOLUTION

Step 1. Let $\mathbf{v}_1 = \mathbf{x}_1$ and $W_1 = \text{Span}\,\{\mathbf{x}_1\} = \text{Span}\,\{\mathbf{v}_1\}$.

Step 2. Let $\mathbf{v}_2$ be the vector produced by subtracting from $\mathbf{x}_2$ its projection onto the subspace W_1. That is, let

$$\begin{aligned} \mathbf{v}_2 &= \mathbf{x}_2 - \text{proj}_{W_1}\mathbf{x}_2 \\ &= \mathbf{x}_2 - \frac{\mathbf{x}_2 \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1}\mathbf{v}_1 \qquad \text{Since } \mathbf{v}_1 = \mathbf{x}_1 \\ &= \begin{bmatrix} 0 \\ 1 \\ 1 \\ 1 \end{bmatrix} - \frac{3}{4}\begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} -3/4 \\ 1/4 \\ 1/4 \\ 1/4 \end{bmatrix} \end{aligned}$$

As in Example 1, $\mathbf{v}_2$ is the component of $\mathbf{x}_2$ orthogonal to $\mathbf{x}_1$, and $\{\mathbf{v}_1, \mathbf{v}_2\}$ is an orthogonal basis for the subspace W_2 spanned by $\mathbf{x}_1$ and $\mathbf{x}_2$.

Step 2′ (optional). If appropriate, scale $\mathbf{v}_2$ to simplify later computations. Since $\mathbf{v}_2$ has fractional entries, it is convenient to scale it by a factor of 4 and replace $\{\mathbf{v}_1, \mathbf{v}_2\}$ by the orthogonal basis

$$\mathbf{v}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \quad \mathbf{v}_2' = \begin{bmatrix} -3 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

Step 3. Let $\mathbf{v}_3$ be the vector produced by subtracting from $\mathbf{x}_3$ its projection onto the subspace W_2. Use the orthogonal basis $\{\mathbf{v}_1, \mathbf{v}_2'\}$ to compute this projection onto W_2:

$$\text{proj}_{W_2}\,\mathbf{x}_3 = \overbrace{\frac{\mathbf{x}_3 \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1}\mathbf{v}_1}^{\substack{\text{Projection of} \\ \mathbf{x}_3 \text{ onto } \mathbf{v}_1}} + \overbrace{\frac{\mathbf{x}_3 \cdot \mathbf{v}_2'}{\mathbf{v}_2' \cdot \mathbf{v}_2'}\mathbf{v}_2'}^{\substack{\text{Projection of} \\ \mathbf{x}_3 \text{ onto } \mathbf{v}_2'}} = \frac{2}{4}\begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} + \frac{2}{12}\begin{bmatrix} -3 \\ 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 2/3 \\ 2/3 \\ 2/3 \end{bmatrix}$$

Then $\mathbf{v}_3$ is the component of $\mathbf{x}_3$ orthogonal to W_2, namely,

$$\mathbf{v}_3 = \mathbf{x}_3 - \text{proj}_{W_2}\,\mathbf{x}_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix} - \begin{bmatrix} 0 \\ 2/3 \\ 2/3 \\ 2/3 \end{bmatrix} = \begin{bmatrix} 0 \\ -2/3 \\ 1/3 \\ 1/3 \end{bmatrix}$$

See Fig. 2 for a diagram of this construction. Observe that $\mathbf{v}_3$ is in W, because $\mathbf{x}_3$ and $\text{proj}_{W_2}\mathbf{x}_3$ are both in W. Thus $\{\mathbf{v}_1, \mathbf{v}_2', \mathbf{v}_3\}$ is an orthogonal set of nonzero vectors and hence a linearly independent set in W. Note that W is three-dimensional since it was defined by a basis of three vectors. Hence, by the Basis Theorem in Section 4.5, $\{\mathbf{v}_1, \mathbf{v}_2', \mathbf{v}_3\}$ is an orthogonal basis for W. ■

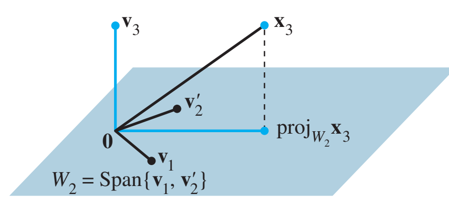


FIGURE 2 The construction of $\mathbf{v}_3$ from $\mathbf{x}_3$ and W_2.

The proof of the next theorem shows that this strategy really works. Scaling of vectors is not mentioned because that is used only to simplify hand calculations.

THEOREM 11

The Gram–Schmidt Process

Given a basis $\{\mathbf{x}_1, \dots, \mathbf{x}_p\}$ for a nonzero subspace W of $\mathbb{R}^n$, define

$$\begin{aligned}
\mathbf{v}_1 &= \mathbf{x}_1 \\
\mathbf{v}_2 &= \mathbf{x}_2 - \frac{\mathbf{x}_2 \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1}\mathbf{v}_1 \\
\mathbf{v}_3 &= \mathbf{x}_3 - \frac{\mathbf{x}_3 \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1}\mathbf{v}_1 - \frac{\mathbf{x}_3 \cdot \mathbf{v}_2}{\mathbf{v}_2 \cdot \mathbf{v}_2}\mathbf{v}_2 \\
&\ \vdots \\
\mathbf{v}_p &= \mathbf{x}_p - \frac{\mathbf{x}_p \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1}\mathbf{v}_1 - \frac{\mathbf{x}_p \cdot \mathbf{v}_2}{\mathbf{v}_2 \cdot \mathbf{v}_2}\mathbf{v}_2 - \cdots - \frac{\mathbf{x}_p \cdot \mathbf{v}_{p-1}}{\mathbf{v}_{p-1} \cdot \mathbf{v}_{p-1}}\mathbf{v}_{p-1}
\end{aligned}$$

Then $\{\mathbf{v}_1, \dots, \mathbf{v}_p\}$ is an orthogonal basis for W. In addition

$$\text{Span}\,\{\mathbf{v}_1, \dots, \mathbf{v}_k\} = \text{Span}\,\{\mathbf{x}_1, \dots, \mathbf{x}_k\} \qquad \text{for } 1 \le k \le p \tag{1}$$

PROOF For $1 \leq k \leq p$, let $W_k = \text{Span}\{\mathbf{x}_1, \dots, \mathbf{x}_k\}$. Set $\mathbf{v}_1 = \mathbf{x}_1$, so that $\text{Span}\{\mathbf{v}_1\} = \text{Span}\{\mathbf{x}_1\}$. Suppose, for some $k < p$, we have constructed $\mathbf{v}_1, \dots, \mathbf{v}_k$ so that $\{\mathbf{v}_1, \dots, \mathbf{v}_k\}$ is an orthogonal basis for W_k. Define

$$\mathbf{v}_{k+1} = \mathbf{x}_{k+1} - \text{proj}_{W_k} \mathbf{x}_{k+1} \tag{2}$$

By the Orthogonal Decomposition Theorem, $\mathbf{v}_{k+1}$ is orthogonal to W_k. Note that $\text{proj}_{W_k} \mathbf{x}_{k+1}$ is in W_k and hence also in W_{k+1}. Since $\mathbf{x}_{k+1}$ is in W_{k+1}, so is $\mathbf{v}_{k+1}$ (because W_{k+1} is a subspace and is closed under subtraction). Furthermore, $\mathbf{v}_{k+1} \neq \mathbf{0}$ because $\mathbf{x}_{k+1}$ is not in $W_k = \text{Span}\{\mathbf{x}_1, \dots, \mathbf{x}_k\}$. Hence $\{\mathbf{v}_1, \dots, \mathbf{v}_{k+1}\}$ is an orthogonal set of nonzero vectors in the $(k+1)$-dimensional space W_{k+1}. By the Basis Theorem in Section 4.5, this set is an orthogonal basis for W_{k+1}. Hence $W_{k+1} = \text{Span}\{\mathbf{v}_1, \dots, \mathbf{v}_{k+1}\}$. When $k + 1 = p$, the process stops. ■

Theorem 11 shows that any nonzero subspace W of $\mathbb{R}^n$ has an orthogonal basis, because an ordinary basis $\{\mathbf{x}_1, \dots, \mathbf{x}_p\}$ is always available (by Theorem 11 in Section 4.5), and the Gram–Schmidt process depends only on the existence of orthogonal projections onto subspaces of W that already have orthogonal bases.

Orthonormal Bases

An orthonormal basis is constructed easily from an orthogonal basis $\{\mathbf{v}_1, \dots, \mathbf{v}_p\}$: simply normalize (i.e., "scale") all the $\mathbf{v}_k$. When working problems by hand, this is easier than normalizing each $\mathbf{v}_k$ as soon as it is found (because it avoids unnecessary writing of square roots).

EXAMPLE 3 Example 1 constructed the orthogonal basis

$$\mathbf{v}_1 = \begin{bmatrix} 3 \\ 6 \\ 0 \end{bmatrix}, \quad \mathbf{v}_2 = \begin{bmatrix} 0 \\ 0 \\ 2 \end{bmatrix}$$

An orthonormal basis is

$$\mathbf{u}_1 = \frac{1}{\|\mathbf{v}_1\|}\mathbf{v}_1 = \frac{1}{\sqrt{45}}\begin{bmatrix} 3 \\ 6 \\ 0 \end{bmatrix} = \begin{bmatrix} 1/\sqrt{5} \\ 2/\sqrt{5} \\ 0 \end{bmatrix}$$

$$\mathbf{u}_2 = \frac{1}{\|\mathbf{v}_2\|}\mathbf{v}_2 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$ ■

QR Factorization of Matrices

WEB

If an $m \times n$ matrix A has linearly independent columns $\mathbf{x}_1, \dots, \mathbf{x}_n$, then applying the Gram–Schmidt process (with normalizations) to $\mathbf{x}_1, \dots, \mathbf{x}_n$ amounts to *factoring* A, as described in the next theorem. This factorization is widely used in computer algorithms for various computations, such as solving equations (discussed in Section 6.5) and finding eigenvalues (mentioned in the exercises for Section 5.2).

THEOREM 12

The QR Factorization

If A is an $m \times n$ matrix with linearly independent columns, then A can be factored as $A = QR$, where Q is an $m \times n$ matrix whose columns form an orthonormal basis for Col A and R is an $n \times n$ upper triangular invertible matrix with positive entries on its diagonal.

PROOF The columns of A form a basis $\{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ for Col A. Construct an orthonormal basis $\{\mathbf{u}_1, \dots, \mathbf{u}_n\}$ for $W = \text{Col } A$ with property (1) in Theorem 11. This basis may be constructed by the Gram–Schmidt process or some other means. Let

$$Q = [\, \mathbf{u}_1 \quad \mathbf{u}_2 \quad \cdots \quad \mathbf{u}_n \,]$$

For $k = 1, \dots, n, \mathbf{x}_k$ is in Span $\{\mathbf{x}_1, \dots, \mathbf{x}_k\} = \text{Span}\,\{\mathbf{u}_1, \dots, \mathbf{u}_k\}$. So there are constants, $r_{1k}, \dots, r_{kk}$, such that

$$\mathbf{x}_k = r_{1k}\mathbf{u}_1 + \cdots + r_{kk}\mathbf{u}_k + 0 \cdot \mathbf{u}_{k+1} + \cdots + 0 \cdot \mathbf{u}_n$$

We may assume that $r_{kk} \geq 0$. (If $r_{kk} < 0$, multiply both r_{kk} and $\mathbf{u}_k$ by -1.) This shows that $\mathbf{x}_k$ is a linear combination of the columns of Q using as weights the entries in the vector

$$\mathbf{r}_k = \begin{bmatrix} r_{1k} \\ \vdots \\ r_{kk} \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

That is, $\mathbf{x}_k = Q\mathbf{r}_k$ for $k = 1, \dots, n$. Let $R = [\, \mathbf{r}_1 \quad \cdots \quad \mathbf{r}_n \,]$. Then

$$A = [\, \mathbf{x}_1 \quad \cdots \quad \mathbf{x}_n \,] = [\, Q\mathbf{r}_1 \quad \cdots \quad Q\mathbf{r}_n \,] = QR$$

The fact that R is invertible follows easily from the fact that the columns of A are linearly independent (Exercise 19). Since R is clearly upper triangular, its nonnegative diagonal entries must be positive. ■

EXAMPLE 4 Find a QR factorization of $A = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$.

SOLUTION The columns of A are the vectors $\mathbf{x}_1$, $\mathbf{x}_2$, and $\mathbf{x}_3$ in Example 2. An orthogonal basis for Col $A = \text{Span}\,\{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3\}$ was found in that example:

$$\mathbf{v}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \quad \mathbf{v}_2' = \begin{bmatrix} -3 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \quad \mathbf{v}_3 = \begin{bmatrix} 0 \\ -2/3 \\ 1/3 \\ 1/3 \end{bmatrix}$$

To simplify the arithmetic that follows, scale $\mathbf{v}_3$ by letting $\mathbf{v}_3' = 3\mathbf{v}_3$. Then normalize the three vectors to obtain $\mathbf{u}_1$, $\mathbf{u}_2$, and $\mathbf{u}_3$, and use these vectors as the columns of Q:

$$Q = \begin{bmatrix} 1/2 & -3/\sqrt{12} & 0 \\ 1/2 & 1/\sqrt{12} & -2/\sqrt{6} \\ 1/2 & 1/\sqrt{12} & 1/\sqrt{6} \\ 1/2 & 1/\sqrt{12} & 1/\sqrt{6} \end{bmatrix}$$

By construction, the first k columns of Q are an orthonormal basis of Span $\{\mathbf{x}_1, \dots, \mathbf{x}_k\}$. From the proof of Theorem 12, $A = QR$ for some R. To find R, observe that $Q^TQ = I$, because the columns of Q are orthonormal. Hence

$$Q^TA = Q^T(QR) = IR = R$$

and

$$R = \begin{bmatrix} 1/2 & 1/2 & 1/2 & 1/2 \\ -3/\sqrt{12} & 1/\sqrt{12} & 1/\sqrt{12} & 1/\sqrt{12} \\ 0 & -2/\sqrt{6} & 1/\sqrt{6} & 1/\sqrt{6} \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} 2 & 3/2 & 1 \\ 0 & 3/\sqrt{12} & 2/\sqrt{12} \\ 0 & 0 & 2/\sqrt{6} \end{bmatrix}$$

■

NUMERICAL NOTES

1. When the Gram–Schmidt process is run on a computer, roundoff error can build up as the vectors $\mathbf{u}_k$ are calculated, one by one. For j and k large but unequal, the inner products $\mathbf{u}_j^T\mathbf{u}_k$ may not be sufficiently close to zero. This loss of orthogonality can be reduced substantially by rearranging the order of the calculations.[1] However, a different computer-based QR factorization is usually preferred to this modified Gram–Schmidt method because it yields a more accurate orthonormal basis, even though the factorization requires about twice as much arithmetic.
2. To produce a QR factorization of a matrix A, a computer program usually left-multiplies A by a sequence of orthogonal matrices until A is transformed into an upper triangular matrix. This construction is analogous to the left-multiplication by elementary matrices that produces an LU factorization of A.

PRACTICE PROBLEM

Let $W = \text{Span}\,\{\mathbf{x}_1, \mathbf{x}_2\}$, where $\mathbf{x}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$ and $\mathbf{x}_2 = \begin{bmatrix} 1/3 \\ 1/3 \\ -2/3 \end{bmatrix}$. Construct an orthonormal basis for W.

6.4 EXERCISES

In Exercises 1–6, the given set is a basis for a subspace W. Use the Gram–Schmidt process to produce an orthogonal basis for W.

1. $\begin{bmatrix} 3 \\ 0 \\ -1 \end{bmatrix}, \begin{bmatrix} 8 \\ 5 \\ -6 \end{bmatrix}$

2. $\begin{bmatrix} 0 \\ 4 \\ 2 \end{bmatrix}, \begin{bmatrix} 5 \\ 6 \\ -7 \end{bmatrix}$

3. $\begin{bmatrix} 2 \\ -5 \\ 1 \end{bmatrix}, \begin{bmatrix} 4 \\ -1 \\ 2 \end{bmatrix}$

4. $\begin{bmatrix} 3 \\ -4 \\ 5 \end{bmatrix}, \begin{bmatrix} -3 \\ 14 \\ -7 \end{bmatrix}$

5. $\begin{bmatrix} 1 \\ -4 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 7 \\ -7 \\ -4 \\ 1 \end{bmatrix}$

6. $\begin{bmatrix} 3 \\ -1 \\ 2 \\ -1 \end{bmatrix}, \begin{bmatrix} -5 \\ 9 \\ -9 \\ 3 \end{bmatrix}$

[1] See *Fundamentals of Matrix Computations*, by David S. Watkins (New York: John Wiley & Sons, 1991), pp. 167–180.

7. Find an orthonormal basis of the subspace spanned by the vectors in Exercise 3.

8. Find an orthonormal basis of the subspace spanned by the vectors in Exercise 4.

Find an orthogonal basis for the column space of each matrix in Exercises 9–12.

9. $\begin{bmatrix} 3 & -5 & 1 \\ 1 & 1 & 1 \\ -1 & 5 & -2 \\ 3 & -7 & 8 \end{bmatrix}$ **10.** $\begin{bmatrix} -1 & 6 & 6 \\ 3 & -8 & 3 \\ 1 & -2 & 6 \\ 1 & -4 & -3 \end{bmatrix}$

11. $\begin{bmatrix} 1 & 2 & 5 \\ -1 & 1 & -4 \\ -1 & 4 & -3 \\ 1 & -4 & 7 \\ 1 & 2 & 1 \end{bmatrix}$ **12.** $\begin{bmatrix} 1 & 3 & 5 \\ -1 & -3 & 1 \\ 0 & 2 & 3 \\ 1 & 5 & 2 \\ 1 & 5 & 8 \end{bmatrix}$

In Exercises 13 and 14, the columns of Q were obtained by applying the Gram–Schmidt process to the columns of A. Find an upper triangular matrix R such that $A = QR$. Check your work.

13. $A = \begin{bmatrix} 5 & 9 \\ 1 & 7 \\ -3 & -5 \\ 1 & 5 \end{bmatrix}, Q = \begin{bmatrix} 5/6 & -1/6 \\ 1/6 & 5/6 \\ -3/6 & 1/6 \\ 1/6 & 3/6 \end{bmatrix}$

14. $A = \begin{bmatrix} -2 & 3 \\ 5 & 7 \\ 2 & -2 \\ 4 & 6 \end{bmatrix}, Q = \begin{bmatrix} -2/7 & 5/7 \\ 5/7 & 2/7 \\ 2/7 & -4/7 \\ 4/7 & 2/7 \end{bmatrix}$

15. Find a QR factorization of the matrix in Exercise 11.

16. Find a QR factorization of the matrix in Exercise 12.

In Exercises 17 and 18, all vectors and subspaces are in $\mathbb{R}^n$. Mark each statement True or False. Justify each answer.

17. a. If $\{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3\}$ is an orthogonal basis for W, then multiplying $\mathbf{v}_3$ by a scalar c gives a new orthogonal basis $\{\mathbf{v}_1, \mathbf{v}_2, c\mathbf{v}_3\}$.

b. The Gram–Schmidt process produces from a linearly independent set $\{\mathbf{x}_1, \dots, \mathbf{x}_p\}$ an orthogonal set $\{\mathbf{v}_1, \dots, \mathbf{v}_p\}$ with the property that for each k, the vectors $\mathbf{v}_1, \dots, \mathbf{v}_k$ span the same subspace as that spanned by $\mathbf{x}_1, \dots, \mathbf{x}_k$.

c. If $A = QR$, where Q has orthonormal columns, then $R = Q^T A$.

18. a. If $W = \text{Span}\,\{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3\}$ with $\{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3\}$ linearly independent, and if $\{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3\}$ is an orthogonal set in W, then $\{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3\}$ is a basis for W.

b. If $\mathbf{x}$ is not in a subspace W, then $\mathbf{x} - \text{proj}_W\, \mathbf{x}$ is not zero.

c. In a QR factorization, say $A = QR$ (when A has linearly independent columns), the columns of Q form an orthonormal basis for the column space of A.

19. Suppose $A = QR$, where Q is $m \times n$ and R is $n \times n$. Show that if the columns of A are linearly independent, then R must be invertible. [*Hint:* Study the equation $R\mathbf{x} = \mathbf{0}$ and use the fact that $A = QR$.]

20. Suppose $A = QR$, where R is an invertible matrix. Show that A and Q have the same column space. [*Hint:* Given $\mathbf{y}$ in Col A, show that $\mathbf{y} = Q\mathbf{x}$ for some $\mathbf{x}$. Also, given $\mathbf{y}$ in Col Q, show that $\mathbf{y} = A\mathbf{x}$ for some $\mathbf{x}$.]

21. Given $A = QR$ as in Theorem 12, describe how to find an orthogonal $m \times m$ (square) matrix Q_1 and an invertible $n \times n$ upper triangular matrix R such that

$$A = Q_1 \begin{bmatrix} R \\ 0 \end{bmatrix}$$

The MATLAB `qr` command supplies this "full" QR factorization when rank $A = n$.

22. Let $\mathbf{u}_1, \dots, \mathbf{u}_p$ be an orthogonal basis for a subspace W of $\mathbb{R}^n$, and let $T : \mathbb{R}^n \to \mathbb{R}^n$ be defined by $T(\mathbf{x}) = \text{proj}_W\, \mathbf{x}$. Show that T is a linear transformation.

23. Suppose $A = QR$ is a QR factorization of an $m \times n$ matrix A (with linearly independent columns). Partition A as $[A_1 \quad A_2]$, where A_1 has p columns. Show how to obtain a QR factorization of A_1, and explain why your factorization has the appropriate properties.

24. [**M**] Use the Gram–Schmidt process as in Example 2 to produce an orthogonal basis for the column space of

$$A = \begin{bmatrix} -10 & 13 & 7 & -11 \\ 2 & 1 & -5 & 3 \\ -6 & 3 & 13 & -3 \\ 16 & -16 & -2 & 5 \\ 2 & 1 & -5 & -7 \end{bmatrix}$$

25. [**M**] Use the method in this section to produce a QR factorization of the matrix in Exercise 24.

26. [**M**] For a matrix program, the Gram–Schmidt process works better with orthonormal vectors. Starting with $\mathbf{x}_1, \dots, \mathbf{x}_p$ as in Theorem 11, let $A = [\,\mathbf{x}_1 \ \cdots \ x_p\,]$. Suppose Q is an $n \times k$ matrix whose columns form an orthonormal basis for the subspace W_k spanned by the first k columns of A. Then for $\mathbf{x}$ in $\mathbb{R}^n$, $QQ^T\mathbf{x}$ is the orthogonal projection of $\mathbf{x}$ onto W_k (Theorem 10 in Section 6.3). If $\mathbf{x}_{k+1}$ is the next column of A, then equation (2) in the proof of Theorem 11 becomes

$$\mathbf{v}_{k+1} = \mathbf{x}_{k+1} - Q(Q^T\mathbf{x}_{k+1})$$

(The parentheses above reduce the number of arithmetic operations.) Let $\mathbf{u}_{k+1} = \mathbf{v}_{k+1}/\|\mathbf{v}_{k+1}\|$. The new Q for the next step is $[\,Q \quad \mathbf{u}_{k+1}\,]$. Use this procedure to compute the QR factorization of the matrix in Exercise 24. Write the keystrokes or commands you use.

WEB

SOLUTION TO PRACTICE PROBLEM

Let $\mathbf{v}_1 = \mathbf{x}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$ and $\mathbf{v}_2 = \mathbf{x}_2 - \dfrac{\mathbf{x}_2 \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1}\mathbf{v}_1 = \mathbf{x}_2 - 0\mathbf{v}_1 = \mathbf{x}_2$. So $\{\mathbf{x}_1, \mathbf{x}_2\}$ is already orthogonal. All that is needed is to normalize the vectors. Let

$$\mathbf{u}_1 = \frac{1}{\|\mathbf{v}_1\|}\mathbf{v}_1 = \frac{1}{\sqrt{3}}\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 1/\sqrt{3} \\ 1/\sqrt{3} \\ 1/\sqrt{3} \end{bmatrix}$$

Instead of normalizing $\mathbf{v}_2$ directly, normalize $\mathbf{v}_2' = 3\mathbf{v}_2$ instead:

$$\mathbf{u}_2 = \frac{1}{\|\mathbf{v}_2'\|}\mathbf{v}_2' = \frac{1}{\sqrt{1^2 + 1^2 + (-2)^2}}\begin{bmatrix} 1 \\ 1 \\ -2 \end{bmatrix} = \begin{bmatrix} 1/\sqrt{6} \\ 1/\sqrt{6} \\ -2/\sqrt{6} \end{bmatrix}$$

Then $\{\mathbf{u}_1, \mathbf{u}_2\}$ is an orthonormal basis for W.

6.5 LEAST-SQUARES PROBLEMS

The chapter's introductory example described a massive problem $A\mathbf{x} = \mathbf{b}$ that had no solution. Inconsistent systems arise often in applications, though usually not with such an enormous coefficient matrix. When a solution is demanded and none exists, the best one can do is to find an $\mathbf{x}$ that makes $A\mathbf{x}$ as close as possible to $\mathbf{b}$.

Think of $A\mathbf{x}$ as an *approximation* to $\mathbf{b}$. The smaller the distance between $\mathbf{b}$ and $A\mathbf{x}$, given by $\|\mathbf{b} - A\mathbf{x}\|$, the better the approximation. The **general least-squares problem** is to find an $\mathbf{x}$ that makes $\|\mathbf{b} - A\mathbf{x}\|$ as small as possible. The adjective "least-squares" arises from the fact that $\|\mathbf{b} - A\mathbf{x}\|$ is the square root of a sum of squares.

DEFINITION

If A is $m \times n$ and $\mathbf{b}$ is in $\mathbb{R}^m$, a **least-squares solution** of $A\mathbf{x} = \mathbf{b}$ is an $\hat{\mathbf{x}}$ in $\mathbb{R}^n$ such that

$$\|\mathbf{b} - A\hat{\mathbf{x}}\| \leq \|\mathbf{b} - A\mathbf{x}\|$$

for all $\mathbf{x}$ in $\mathbb{R}^n$.

The most important aspect of the least-squares problem is that no matter what $\mathbf{x}$ we select, the vector $A\mathbf{x}$ will necessarily be in the column space, Col A. So we seek an $\mathbf{x}$ that makes $A\mathbf{x}$ the closest point in Col A to $\mathbf{b}$. See Fig. 1. (Of course, if $\mathbf{b}$ happens to be in Col A, then $\mathbf{b}$ *is* $A\mathbf{x}$ for some $\mathbf{x}$, and such an $\mathbf{x}$ is a "least-squares solution.")

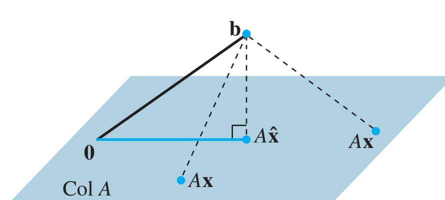


FIGURE 1 The vector $\mathbf{b}$ is closer to $A\hat{\mathbf{x}}$ than to $A\mathbf{x}$ for other $\mathbf{x}$.

Fourier Series (Calculus required)

Continuous functions are often approximated by linear combinations of sine and cosine functions. For instance, a continuous function might represent a sound wave, an electric signal of some type, or the movement of a vibrating mechanical system.

For simplicity, we consider functions on $0 \le t \le 2\pi$. It turns out that any function in $C[0, 2\pi]$ can be approximated as closely as desired by a function of the form

$$\frac{a_0}{2} + a_1 \cos t + \cdots + a_n \cos nt + b_1 \sin t + \cdots + b_n \sin nt \tag{4}$$

for a sufficiently large value of n. The function (4) is called a **trigonometric polynomial**. If a_n and b_n are not both zero, the polynomial is said to be of **order n**. The connection between trigonometric polynomials and other functions in $C[0, 2\pi]$ depends on the fact that for any $n \ge 1$, the set

$$\{1, \cos t, \cos 2t, \ldots, \cos nt, \sin t, \sin 2t, \ldots, \sin nt\} \tag{5}$$

is orthogonal with respect to the inner product

$$\langle f, g \rangle = \int_0^{2\pi} f(t)g(t)\,dt \tag{6}$$

This orthogonality is verified as in the following example and in Exercises 5 and 6.

EXAMPLE 3 Let $C[0, 2\pi]$ have the inner product (6), and let m and n be unequal positive integers. Show that $\cos mt$ and $\cos nt$ are orthogonal.

SOLUTION Use a trigonometric identity. When $m \ne n$,

$$\begin{aligned}\langle \cos mt, \cos nt \rangle &= \int_0^{2\pi} \cos mt \cos nt\,dt \\ &= \frac{1}{2}\int_0^{2\pi} [\cos(mt + nt) + \cos(mt - nt)]\,dt \\ &= \frac{1}{2}\left[\frac{\sin(mt+nt)}{m+n} + \frac{\sin(mt-nt)}{m-n}\right]\Bigg|_0^{2\pi} = 0\end{aligned}$$

Let W be the subspace of $C[0, 2\pi]$ spanned by the functions in (5). Given f in $C[0, 2\pi]$, the best approximation to f by functions in W is called the ***n*th-order Fourier approximation** to f on $[0, 2\pi]$. Since the functions in (5) are orthogonal, the best approximation is given by the orthogonal projection onto W. In this case, the coefficients a_k and b_k in (4) are called the **Fourier coefficients** of f. The standard formula for an orthogonal projection shows that

$$a_k = \frac{\langle f, \cos kt \rangle}{\langle \cos kt, \cos kt \rangle}, \quad b_k = \frac{\langle f, \sin kt \rangle}{\langle \sin kt, \sin kt \rangle}, \quad k \ge 1$$

Exercise 7 asks you to show that $\langle \cos kt, \cos kt \rangle = \pi$ and $\langle \sin kt, \sin kt \rangle = \pi$. Thus

$$a_k = \frac{1}{\pi}\int_0^{2\pi} f(t)\cos kt\,dt, \quad b_k = \frac{1}{\pi}\int_0^{2\pi} f(t)\sin kt\,dt \tag{7}$$

The coefficient of the (constant) function 1 in the orthogonal projection is

$$\frac{\langle f, 1 \rangle}{\langle 1, 1 \rangle} = \frac{1}{2\pi}\int_0^{2\pi} f(t)\cdot 1\,dt = \frac{1}{2}\left[\frac{1}{\pi}\int_0^{2\pi} f(t)\cos(0\cdot t)\,dt\right] = \frac{a_0}{2}$$

where a_0 is defined by (7) for $k = 0$. This explains why the constant term in (4) is written as $a_0/2$.

EXAMPLE 4 Find the nth-order Fourier approximation to the function $f(t) = t$ on the interval $[0, 2\pi]$.

SOLUTION Compute

$$\frac{a_0}{2} = \frac{1}{2}\cdot\frac{1}{\pi}\int_0^{2\pi} t\,dt = \frac{1}{2\pi}\left[\frac{1}{2}t^2\Big|_0^{2\pi}\right] = \pi$$

and for $k > 0$, using integration by parts,

$$a_k = \frac{1}{\pi}\int_0^{2\pi} t\cos kt\,dt = \frac{1}{\pi}\left[\frac{1}{k^2}\cos kt + \frac{t}{k}\sin kt\right]_0^{2\pi} = 0$$

$$b_k = \frac{1}{\pi}\int_0^{2\pi} t\sin kt\,dt = \frac{1}{\pi}\left[\frac{1}{k^2}\sin kt - \frac{t}{k}\cos kt\right]_0^{2\pi} = -\frac{2}{k}$$

Thus the nth-order Fourier approximation of $f(t) = t$ is

$$\pi - 2\sin t - \sin 2t - \frac{2}{3}\sin 3t - \cdots - \frac{2}{n}\sin nt$$

Figure 3 shows the third- and fourth-order Fourier approximations of f. ■

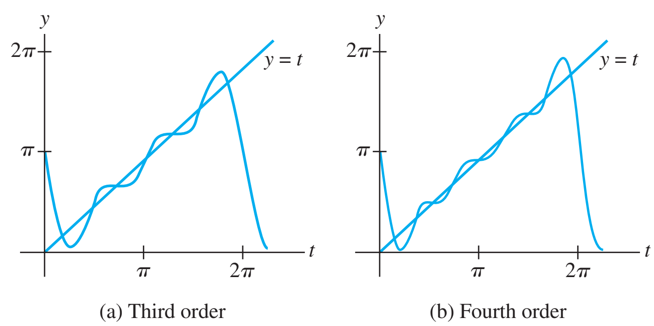


FIGURE 3 Fourier approximations of the function $f(t) = t$.

The norm of the difference between f and a Fourier approximation is called the **mean square error** in the approximation. (The term *mean* refers to the fact that the norm is determined by an integral.) It can be shown that the mean square error approaches zero as the order of the Fourier approximation increases. For this reason, it is common to write

$$f(t) = \frac{a_0}{2} + \sum_{m=1}^{\infty}(a_m\cos mt + b_m\sin mt)$$

This expression for $f(t)$ is called the **Fourier series** for f on $[0, 2\pi]$. The term $a_m\cos mt$, for example, is the projection of f onto the one-dimensional subspace spanned by $\cos mt$.

PRACTICE PROBLEMS

1. Let $q_1(t) = 1$, $q_2(t) = t$, and $q_3(t) = 3t^2 - 4$. Verify that $\{q_1, q_2, q_3\}$ is an orthogonal set in $C[-2, 2]$ with the inner product of Example 7 in Section 6.7 (integration from -2 to 2).
2. Find the first-order and third-order Fourier approximations to

$$f(t) = 3 - 2\sin t + 5\sin 2t - 6\cos 2t$$

6.8 EXERCISES

1. Find the least-squares line $y = \beta_0 + \beta_1 x$ that best fits the data $(-2, 0)$, $(-1, 0)$, $(0, 2)$, $(1, 4)$, and $(2, 4)$, assuming that the first and last data points are less reliable. Weight them half as much as the three interior points.

2. Suppose 5 out of 25 data points in a weighted least-squares problem have a y-measurement that is less reliable than the others, and they are to be weighted half as much as the other 20 points. One method is to weight the 20 points by a factor of 1 and the other 5 by a factor of $\frac{1}{2}$. A second method is to weight the 20 points by a factor of 2 and the other 5 by a factor of 1. Do the two methods produce different results? Explain.

3. Fit a cubic trend function to the data in Example 2. The orthogonal cubic polynomial is $p_3(t) = \frac{5}{6}t^3 - \frac{17}{6}t$.

4. To make a trend analysis of six evenly spaced data points, one can use orthogonal polynomials with respect to evaluation at the points $t = -5, -3, -1, 1, 3$, and 5.
   a. Show that the first three orthogonal polynomials are
   $$p_0(t) = 1, \quad p_1(t) = t, \quad \text{and} \quad p_2(t) = \tfrac{3}{8}t^2 - \tfrac{35}{8}$$
   (The polynomial p_2 has been scaled so that its values at the evaluation points are small integers.)
   b. Fit a quadratic trend function to the data
   $$(-5, 1), (-3, 1), (-1, 4), (1, 4), (3, 6), (5, 8)$$

In Exercises 5–14, the space is $C[0, 2\pi]$ with the inner product (6).

5. Show that $\sin mt$ and $\sin nt$ are orthogonal when $m \neq n$.

6. Show that $\sin mt$ and $\cos nt$ are orthogonal for all positive integers m and n.

7. Show that $\|\cos kt\|^2 = \pi$ and $\|\sin kt\|^2 = \pi$ for $k > 0$.

8. Find the third-order Fourier approximation to $f(t) = t - 1$.

9. Find the third-order Fourier approximation to $f(t) = 2\pi - t$.

10. Find the third-order Fourier approximation to the *square wave function*, $f(t) = 1$ for $0 \leq t < \pi$ and $f(t) = -1$ for $\pi \leq t < 2\pi$.

11. Find the third-order Fourier approximation to $\sin^2 t$, without performing any integration calculations.

12. Find the third-order Fourier approximation to $\cos^3 t$, without performing any integration calculations.

13. Explain why a Fourier coefficient of the sum of two functions is the sum of the corresponding Fourier coefficients of the two functions.

14. Suppose the first few Fourier coefficients of some function f in $C[0, 2\pi]$ are a_0, a_1, a_2, and b_1, b_2, b_3. Which of the following trigonometric polynomials is closer to f? Defend your answer.
$$g(t) = \frac{a_0}{2} + a_1 \cos t + a_2 \cos 2t + b_1 \sin t$$
$$h(t) = \frac{a_0}{2} + a_1 \cos t + a_2 \cos 2t + b_1 \sin t + b_2 \sin 2t$$

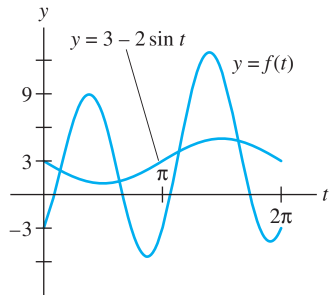
15. **[M]** Refer to the data in Exercise 13 in Section 6.6, concerning the takeoff performance of an airplane. Suppose the possible measurement errors become greater as the speed of the airplane increases, and let W be the diagonal weighting matrix whose diagonal entries are 1, 1, 1, .9, .9, .8, .7, .6, .5, .4, .3, .2, and .1. Find the cubic curve that fits the data with minimum weighted least-squares error, and use it to estimate the velocity of the plane when $t = 4.5$ seconds.

16. **[M]** Let f_4 and f_5 be the fourth-order and fifth-order Fourier approximations in $C[0, 2\pi]$ to the square wave function in Exercise 10. Produce separate graphs of f_4 and f_5 on the interval $[0, 2\pi]$, and produce a graph of f_5 on $[-2\pi, 2\pi]$.

SG The Linearity of an Orthogonal Projection 6–25

SOLUTIONS TO PRACTICE PROBLEMS

1. Compute
$$\langle q_1, q_2 \rangle = \int_{-2}^{2} 1 \cdot t \, dt = \frac{1}{2}t^2 \Big|_{-2}^{2} = 0$$
$$\langle q_1, q_3 \rangle = \int_{-2}^{2} 1 \cdot (3t^2 - 4) \, dt = (t^3 - 4t) \Big|_{-2}^{2} = 0$$
$$\langle q_2, q_3 \rangle = \int_{-2}^{2} t \cdot (3t^2 - 4) \, dt = \left(\frac{3}{4}t^4 - 2t^2 \right) \Big|_{-2}^{2} = 0$$



First- and third-order approximations to $f(t)$.

2. The third-order Fourier approximation to f is the best approximation in $C[0, 2\pi]$ to f by functions (vectors) in the subspace spanned by 1, $\cos t$, $\cos 2t$, $\cos 3t$, $\sin t$, $\sin 2t$, and $\sin 3t$. But f is obviously *in* this subspace, so f is its own best approximation:

$$f(t) = 3 - 2\sin t + 5\sin 2t - 6\cos 2t$$

For the first-order approximation, the closest function to f in the subspace $W = \text{Span}\{1, \cos t, \sin t\}$ is $3 - 2\sin t$. The other two terms in the formula for $f(t)$ are orthogonal to the functions in W, so they contribute nothing to the integrals that give the Fourier coefficients for a first-order approximation.

CHAPTER 6 SUPPLEMENTARY EXERCISES

1. The following statements refer to vectors in $\mathbb{R}^n$ (or $\mathbb{R}^m$) with the standard inner product. Mark each statement True or False. Justify each answer.

a. The length of every vector is a positive number.

b. A vector $\mathbf{v}$ and its negative $-\mathbf{v}$ have equal lengths.

c. The distance between $\mathbf{u}$ and $\mathbf{v}$ is $\|\mathbf{u} - \mathbf{v}\|$.

d. If r is any scalar, then $\|r\mathbf{v}\| = r\|\mathbf{v}\|$.

e. If two vectors are orthogonal, they are linearly independent.

f. If $\mathbf{x}$ is orthogonal to both $\mathbf{u}$ and $\mathbf{v}$, then $\mathbf{x}$ must be orthogonal to $\mathbf{u} - \mathbf{v}$.

g. If $\|\mathbf{u} + \mathbf{v}\|^2 = \|\mathbf{u}\|^2 + \|\mathbf{v}\|^2$, then $\mathbf{u}$ and $\mathbf{v}$ are orthogonal.

h. If $\|\mathbf{u} - \mathbf{v}\|^2 = \|\mathbf{u}\|^2 + \|\mathbf{v}\|^2$, then $\mathbf{u}$ and $\mathbf{v}$ are orthogonal.

i. The orthogonal projection of $\mathbf{y}$ onto $\mathbf{u}$ is a scalar multiple of $\mathbf{y}$.

j. If a vector $\mathbf{y}$ coincides with its orthogonal projection onto a subspace W, then $\mathbf{y}$ is in W.

k. The set of all vectors in $\mathbb{R}^n$ orthogonal to one fixed vector is a subspace of $\mathbb{R}^n$.

l. If W is a subspace of $\mathbb{R}^n$, then W and $W^\perp$ have no vectors in common.

m. If $\{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3\}$ is an orthogonal set and if c_1, c_2, and c_3 are scalars, then $\{c_1\mathbf{v}_1, c_2\mathbf{v}_2, c_3\mathbf{v}_3\}$ is an orthogonal set.

n. If a matrix U has orthonormal columns, then $UU^T = I$.

o. A square matrix with orthogonal columns is an orthogonal matrix.

p. If a square matrix has orthonormal columns, then it also has orthonormal rows.

q. If W is a subspace, then $\|\text{proj}_W \mathbf{v}\|^2 + \|\mathbf{v} - \text{proj}_W \mathbf{v}\|^2 = \|\mathbf{v}\|^2$.

r. A least-squares solution of $A\mathbf{x} = \mathbf{b}$ is the vector $A\hat{\mathbf{x}}$ in Col A closest to $\mathbf{b}$, so that $\|\mathbf{b} - A\hat{\mathbf{x}}\| \le \|\mathbf{b} - A\mathbf{x}\|$ for all $\mathbf{x}$.

s. The normal equations for a least-squares solution of $A\mathbf{x} = \mathbf{b}$ are given by $\hat{\mathbf{x}} = (A^TA)^{-1}A^T\mathbf{b}$.

2. Let $\{\mathbf{v}_1, \dots, \mathbf{v}_p\}$ be an orthonormal set. Verify the following equality by induction, beginning with $p = 2$. If $\mathbf{x} = c_1\mathbf{v}_1 + \cdots + c_p\mathbf{v}_p$, then

$$\|\mathbf{x}\|^2 = |c_1|^2 + \cdots + |c_p|^2$$

3. Let $\{\mathbf{v}_1, \dots, \mathbf{v}_p\}$ be an orthonormal set in $\mathbb{R}^n$. Verify the following inequality, called *Bessel's inequality*, which is true for each $\mathbf{x}$ in $\mathbb{R}^n$:

$$\|\mathbf{x}\|^2 \ge |\mathbf{x}\cdot\mathbf{v}_1|^2 + |\mathbf{x}\cdot\mathbf{v}_2|^2 + \cdots + |\mathbf{x}\cdot\mathbf{v}_p|^2$$

4. Let U be an $n \times n$ orthogonal matrix. Show that if $\{\mathbf{v}_1, \dots, \mathbf{v}_n\}$ is an orthonormal basis for $\mathbb{R}^n$, then so is $\{U\mathbf{v}_1, \dots, U\mathbf{v}_n\}$.

5. Show that if an $n \times n$ matrix U satisfies $(U\mathbf{x})\cdot(U\mathbf{y}) = \mathbf{x}\cdot\mathbf{y}$ for all $\mathbf{x}$ and $\mathbf{y}$ in $\mathbb{R}^n$, then U is an orthogonal matrix.

6. Show that if U is an orthogonal matrix, then any real eigenvalue of U must be ± 1.

7. A *Householder matrix*, or an *elementary reflector*, has the form $Q = I - 2\mathbf{u}\mathbf{u}^T$ where $\mathbf{u}$ is a unit vector. (See Exercise 13 in the Supplementary Exercises for Chapter 2.) Show that Q is an orthogonal matrix. (Elementary reflectors are often used in computer programs to produce a QR factorization of a matrix A. If A has linearly independent columns, then left-multiplication by a sequence of elementary reflectors can produce an upper triangular matrix.)